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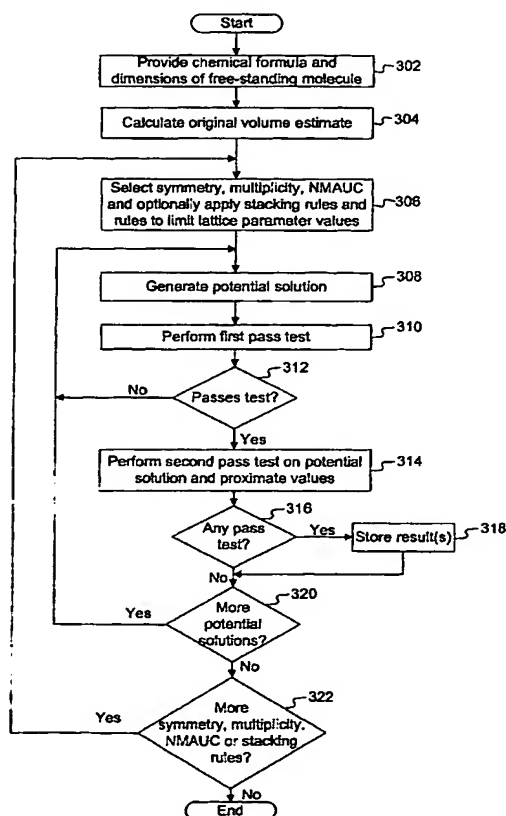
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(54) Title: METHOD FOR MONTE CARLO INDEXING OF POWDER DIFFRACTION DATA



(57) Abstract: Crystalline solid forms may be characterized by their unit cell parameters through a process known as indexing. An embodiment of the invention searches for the unit cell parameters of a crystalline solid form using a Monte-Carlo algorithm that incorporates certain rules to reduce search space. Another embodiment refines the results of the search to identify the correct unit cell parameters of the crystalline solid form. These methods may be automated, conveniently requiring little interaction from the user. The indexing method of the invention may be applied, for example, to distinguish between different crystalline solid forms of a substance.

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